Figure 1

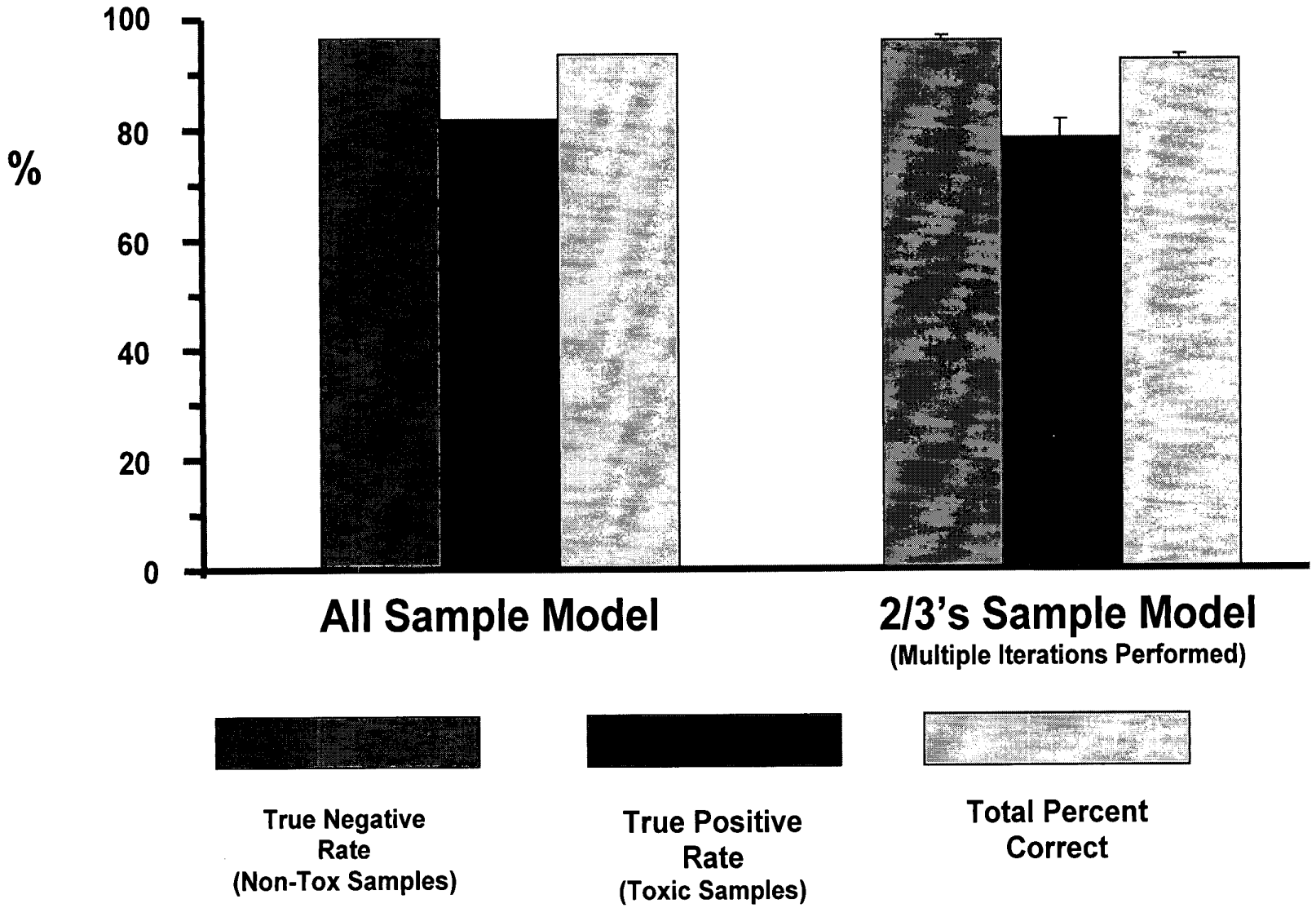

100
80
60
40
20
0
%
All Sample Model
2/3's Sample Model
(Multiple Iterations Performed)
True Negative Rate (Non-Tox Samples)
True Positive Rate (Toxic Samples)
Total Percent Correct

Figure 2

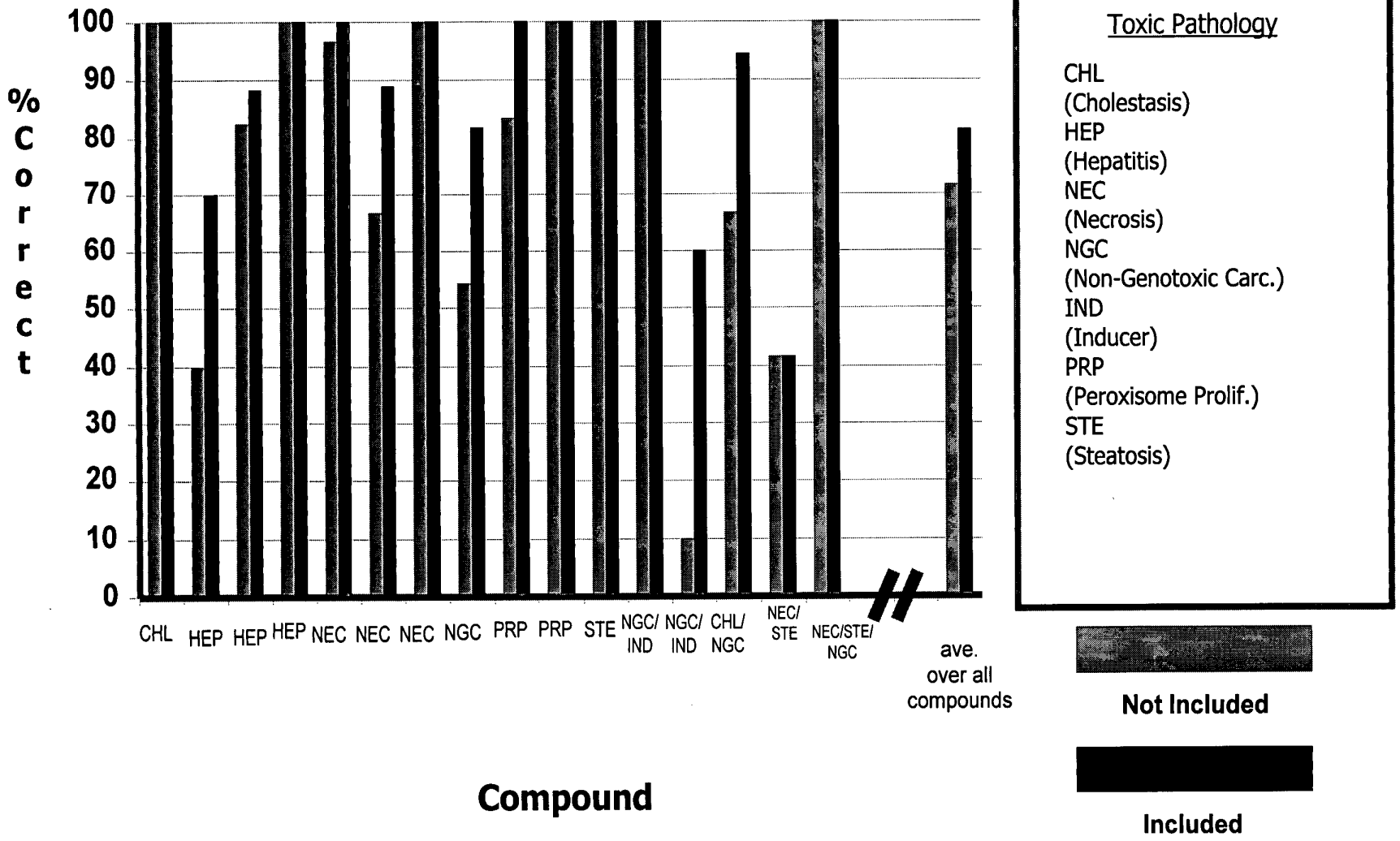
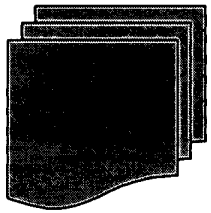
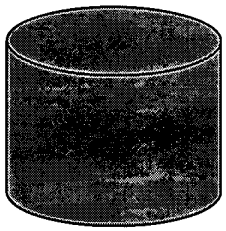

% Correct
100
90
80
70
60
50
40
30
20
10
0
CHL
HEP
HEP
HEP
NEC
NEC
NEC
NGC
PRP
PRP
STE
NGC/ IND
NGC/ IND
CHL/ NGC
NEC/ STE
NEC/STE/ NGC
ave. over all compounds
Compound
Toxic Pathology
CHL
(Cholestasis)
HEP
(Hepatitis)
NEC
(Necrosis)
NGC
(Non-Genotoxic Carc.)
IND
(Inducer)
PRP
(Peroxisome Prolif.)
STE
(Steatosis)
Not Included
Included

Figure 3

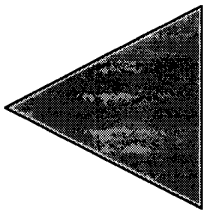


Million +

Data points per study



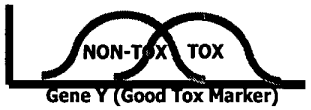
Data base updated daily



Extract sample groups that share toxicity similarities and control groups.

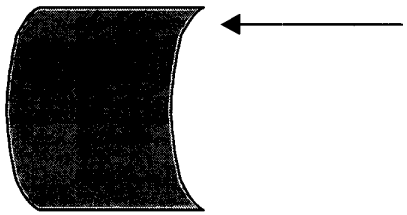
Hundreds of supervised question/models

Optimized LDA method



Need for extensive cross-validation because of over-training minimized

High Speed Selection of markers and robust models.



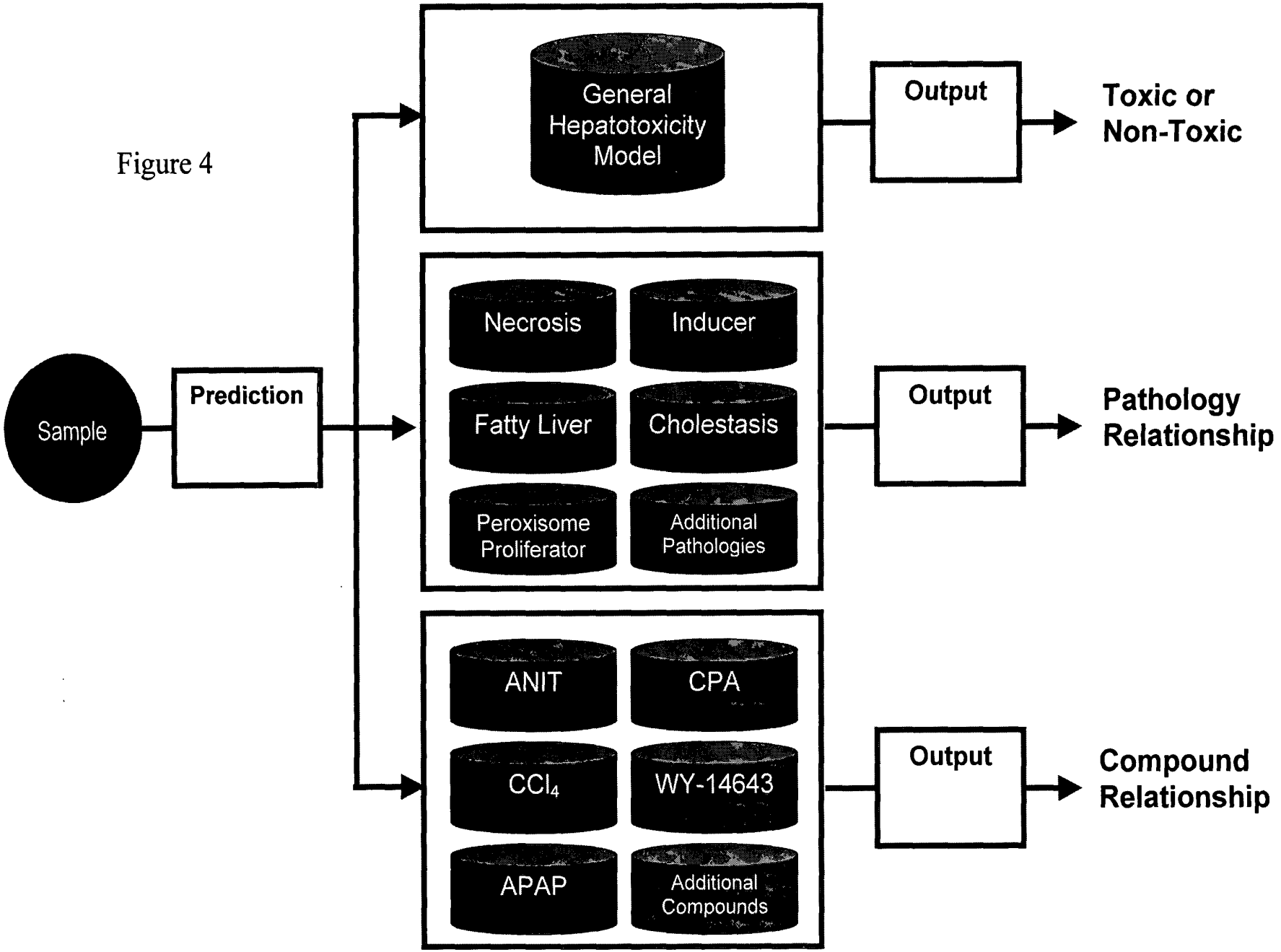
Collection of models and their evaluations

Decision on what new studies to run

Study Results

Several studies per week

Figure 4


General Hepatotoxicity Model
Output
Toxic or Non-Toxic
Necrosis
Inducer
Fatty Liver
Cholestasis
Peroxisome Proliferator
Additional Pathologies
Output
Pathology Relationship
Sample
Prediction
ANIT
CPA
CCl_4
WY-14643
APAP
Additional Compounds
Output
Compound Relationship